

Finite-Temperature Collective Excitations of a Bose-Einstein Condensate

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We derive a simple formula for the finite-temperature shifts of the collective excitations of a Bose-Einstein condensate. To test the validity of our treatment we apply it to explain the anomalous behavior of the “ $m = 2$ ” excitation frequency in the recent JILA experiments (D. S. Jin *et al.*, PRL, **78** (1997) 764), where this frequency does not approach its “noninteracting” value at $\omega = 2\omega_p$, but, instead, decreases with temperature. It turns out that the effect is mainly governed by a resonance between the *condensate* excitation frequency and one of the quantum eigenfrequencies of the *thermal cloud*. Comparison of our predictions with the JILA experimental data shows a good agreement.

The recent discovery of the Bose-Einstein condensation in dilute atomic gases [1] has incurred a tremendous burst of experimental and theoretical research in this area. Whereas zero-temperature properties of Bose condensates seem to be well understood by now, theory of the finite-temperature behavior of the system is far from being complete. One of the most intriguing effects unexplained so far is the shifts in the spectrum of collective excitations at finite temperatures. A possibility of direct comparison of the theoretical predictions in this area with the experimental data [2,3] provides us with a unique opportunity to test the numerous theoretical assumptions used to describe Bose gases in general. Among such open issues are validity of the mean-field description, relevance of the anomalous density of the non-condensed particles, role of the many-body and trap-induced modifications of the interaction strength *etc.*

The first attempt to approach the problem of the finite-temperature shifts was made in the works [4,5] where the collective excitation frequencies were associated with the elementary excitations spectrum of a stationary Popov Hamiltonian, where the thermal cloud was considered as being static. In a subsequent paper [6] the model was improved by taking into account the many-body reduction of the interaction strength [7]. The next important step forward involved the dynamical response of the thermal cloud [8,9]. Furthermore in the Ref. [10] the frequency shifts were calculated using Gaussian *ansatz* for both the condensate and the thermal cloud. Hydrodynamic treatment of the problem is presented in [11]. Whereas all the works listed above were based on the mean-field treatment authors of the paper [12] develop a perturbation theory to derive expressions for both frequencies and damping rates.

In our work we first derive a general formula for the

finite temperature frequency shifts of the collective excitations of a Bose condensate: the expression we obtain is independent of model chosen to describe the thermal cloud. Furthermore we notice that the recent finite-temperature excitation experiments in JILA [2] give us an excellent opportunity to test our findings: using the fact that in the case of the “ $m=2$ ” excitation a strong resonance between the collective excitation of interest and one of the quantum eigenfrequencies of the thermal cloud takes place, we restrict our description of the dynamical response of the thermal cloud to only two modes and obtain a simple closed set of algebraic equations, from which we deduce the values of the frequency shifts at different temperatures. We compare our results with the JILA experimental data.

Let us consider a time-dependent Gross-Pitaevskii-like equation for the mean $\phi = \langle \hat{\psi} \rangle$ of the quantum field $\hat{\psi}$ of a collection of trapped bosons below the Bose-Einstein transition temperature:

$$i\hbar \frac{\partial}{\partial t} \phi = [\frac{p^2}{2M} + V_{\text{trap}} + g(n_c + 2\tilde{n})] \phi + g\tilde{m} \phi^* ; \quad (1)$$

here and below $n_c = N_c|\phi|^2$ and $m_c = N_c\phi^2$ are the condensate normal and “anomalous” densities, N_c is the number of particles in the condensate, $\tilde{n} = \langle \delta\hat{\psi}^\dagger \delta\hat{\psi} \rangle$ and $\tilde{m} = \langle \delta\hat{\psi} \delta\hat{\psi} \rangle$ are the normal and “anomalous” densities of the excited particles expressed through the variance of the field $\delta\hat{\psi} = \hat{\psi} - \langle \hat{\psi} \rangle$, the condensate wave function is supposed to be normalized to unity at the initial instant of time, coupling constant g is defined as $g = 4\pi\hbar^2 a/M$, a is the *s*-wave atomic scattering length, and M is the atomic mass. Note that if the thermal densities \tilde{n} and \tilde{m} are known the above equation is exact [13].

We will be interested in oscillating solutions of (1) whose frequency is close to the frequency $\omega_{\mathbf{k}_{\text{mode}}}$ of the one of the zero-temperature condensate excitations. We will use the following *ansatz*

$$\begin{aligned} \phi(t) &= \left\{ \phi^{(0)} + D\phi^{(-)} e^{-i(\omega_{\mathbf{k}_{\text{mode}}} + \epsilon)t} + D^* \phi^{(+)} e^{+i(\omega_{\mathbf{k}_{\text{mode}}} + \epsilon)t} \right\} \\ &\quad \times e^{-i\mu t} \end{aligned} \quad (2)$$

$$\tilde{n}(t) = \tilde{n}^{(0)} + \tilde{n}^{(-)} e^{-i(\omega_{\mathbf{k}_{\text{mode}}} + \epsilon)t} + \tilde{n}^{(+)} e^{+i(\omega_{\mathbf{k}_{\text{mode}}} + \epsilon)t} \quad (3)$$

$$\tilde{m}(t) = \left\{ \tilde{m}^{(0)} + \tilde{m}^{(-)} e^{-i(\omega_{\mathbf{k}_{\text{mode}}} + \epsilon)t} + \tilde{m}^{(+)} e^{+i(\omega_{\mathbf{k}_{\text{mode}}} + \epsilon)t} \right\} \quad (4)$$

$$\begin{aligned} &\quad \times e^{-2i\mu t} \end{aligned}$$

to describe the motion of the condensate and thermal cloud. Here ϵ is the frequency shift of interest, μ is the chemical potential, and D is the amplitude of the condensate oscillations. We will suppose also that the thermal densities \tilde{n} and \tilde{m} are known functions of the amplitude D :

$$\tilde{n} = \tilde{n}(D) \quad \tilde{m} = \tilde{m}(D) \quad (5)$$

Furthermore we will assume that the oscillations of the thermal density are “induced” by the condensate oscillations and, therefore, the (+)- and (-)-components of the thermal density go to zero as the condensate oscillation amplitude D goes to zero: $\tilde{n}^{(-,+)}(D=0) = \tilde{m}^{(-,+)}(D=0) = 0$.

There are two independent small parameters present in the problem: the ratio between the non-condensed and condensed densities \tilde{n}/n_c and the amplitude D . Let us now expand ϕ , μ , and ϵ into a double series with respect to both \tilde{n}/n_c and D , expand \tilde{n} and \tilde{m} into a simple series with respect to D , and then insert this expansions in the condensate equation (1). To zeroth order in \tilde{n}/n_c and for the infinitely small amplitudes of the condensate oscillations, the stationary part of the condensate wave function is given by the ground state solution Φ of the Gross-Pitaevskii equation

$$\left[\frac{p^2}{2M} + V_{\text{trap}} + gN_c|\Phi|^2 \right] \Phi = \mu_0 \Phi , \quad (6)$$

where the chemical potential μ_0 is chosen in such a way that the condensate wave function is properly normalized: $\langle \Phi | \Phi \rangle = 1$. The oscillating part of the condensate wave function

$$|\phi^{(-/+)}\rangle \doteq \begin{pmatrix} \phi^{(-)} \\ (\phi^{(+)})^* \end{pmatrix} \quad (7)$$

appears only in the first order in D (and zeroth order in \tilde{n}/n_c): it is given by

$$|\phi^{(-/+)}\rangle \approx |W_{\mathbf{k}_{\text{mode}}}\rangle \quad (8)$$

where $|W_{\mathbf{k}_{\text{mode}}}\rangle \doteq (U_{\mathbf{k}_{\text{mode}}}, V_{\mathbf{k}_{\text{mode}}})$ is the mode function of the collective excitation we work with. This mode function is represented by an eigenstate of the Bogoliubov-de-Gennes Liouvillian

$$\mathcal{L}_0 = \begin{pmatrix} L_0 & M_0 \\ -M_0^* & -L_0 \end{pmatrix} \quad (9)$$

$$L_0 = \frac{p^2}{2M} + V_{\text{trap}} + 2gN_c|\Phi|^2 - \mu_0$$

$$M_0 = gN_c\Phi^2$$

of an energy $E_{\mathbf{k}_{\text{mode}}} = \hbar\omega_{\mathbf{k}_{\text{mode}}}$. The eigenstate $|W_{\mathbf{k}_{\text{mode}}}\rangle$ is supposed to be “normalized” to unity: $\langle W_{\mathbf{k}_{\text{mode}}} | W_{\mathbf{k}_{\text{mode}}} \rangle = 1$, where the bilinear form $\langle \cdot | \cdot \rangle$ is defined as

$$\langle W_p | W_q \rangle \doteq \int d^3\mathbf{r} \{ U_p^* U_q - V_p^* V_q \} . \quad (10)$$

Let us now consider the terms of the first order in \tilde{n}/n_c and zeroth order in D in the lhs and rhs of the condensate equation (1). To this order of approximation we can calculate the thermal-cloud-induced correction to the chemical potential $\Delta\mu = \mu - \mu_0$, and it reads

$$\Delta\mu = \langle \Phi_a | \Delta\tilde{\mathcal{L}}_{D=0}^{(0)} | \sigma_3 \Phi \rangle . \quad (11)$$

Note that this correction is given by an off-diagonal matrix element of the stationary part of the thermal correction to the unperturbed Liouvillian $\mathcal{L}^{(0)}$

$$\Delta\tilde{\mathcal{L}}^{(0)} = \begin{pmatrix} 2g\tilde{n}^{(0)} & g\tilde{m}^{(0)} \\ -g(\tilde{m}^{(0)})^* & -2g(\tilde{n}^{(0)}) \end{pmatrix} \quad (12)$$

calculated between the zero-energy “condensate” eigenmode $|\Phi\rangle \doteq (\Phi, -\Phi^*)$ and a state $|\Phi_a\rangle \doteq \sqrt{N_c} \frac{\partial}{\partial N_c} (\sqrt{N_c} \sigma_3 |\Phi\rangle)$ introduced in [14,15] (so-called “lost eigenvector”: it is the only eigenvector of the operator $(\mathcal{L}_0)^2$ not present in the set of the eigenstates of \mathcal{L}_0 itself). The matrix $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the third Pauli matrix.

To the same order in \tilde{n}/n_c and D one can show that the correction to the condensate wave function $\Delta\Phi = \phi^{(0)} - \Phi$ is given by a solution of an inhomogeneous equation

$$\mathcal{L}_0 |\Delta\Phi\rangle = -(\Delta\tilde{\mathcal{L}}_{D=0}^{(0)} - \Delta\mu) |\sigma_3 \Phi\rangle \quad (13)$$

and is a subject of an additional constraint

$$\langle \Phi | \Delta\Phi \rangle = 0 . \quad (14)$$

Here the vector $|\Delta\Phi\rangle$ is defined as $|\Delta\Phi\rangle \doteq (\Delta\Phi, \Delta\Phi^*)$.

Consider now the terms in the equation (1) which are linear with both \tilde{n}/n_c and D . To this order the frequency shift we are interested in is given by

$$\hbar\epsilon = \langle W_{\mathbf{k}_{\text{mode}}} | \Delta\mathcal{L}_c^{(0)} + \Delta\tilde{\mathcal{L}}_{D=0}^{(0)} - \Delta\mu\sigma_3 | W_{\mathbf{k}_{\text{mode}}} \rangle \quad (15)$$

$$+ \langle W_{\mathbf{k}_{\text{mode}}} | \frac{\partial}{\partial D} \Delta\tilde{\mathcal{L}}_{D=0}^{(-/+)} | \sigma_3 \Phi \rangle$$

where the condensate-induced correction to the Liouvillian (9) and the oscillating part of the thermal correction to it read

$$\Delta\mathcal{L}_c = \quad (16)$$

$$\begin{pmatrix} 2g[\Phi^*\Delta\Phi + \Delta\Phi^*\Phi] & 2g\Phi\Delta\Phi \\ -2g\Phi^*\Delta\Phi^* & -2g[\Phi^*\Delta\Phi + \Delta\Phi^*\Phi] \end{pmatrix}$$

$$\Delta\tilde{\mathcal{L}}^{(-/+)} = \begin{pmatrix} 2g\tilde{n}^{(-)} & g\tilde{m}^{(-)} \\ -g(\tilde{m}^{(+)})^* & -2g(\tilde{n}^{(+)})^* \end{pmatrix} \quad (17)$$

respectively. The formulas (11,13,15) defining the finite-temperature frequency shift of the condensate oscillation frequency is the central result of our paper.

In the derivation above we have used a conjecture of completeness of the basis formed by the vectors $\{|\Phi\rangle; |\Phi_a\rangle; |W_{\mathbf{k}}\rangle; |\sigma_1 W_{\mathbf{k}}^*\rangle\}$ (see [15]), where the mode functions $|W_{\mathbf{k}}\rangle$ are the positive energy eigenstates of the unperturbed Liouvillian:

$$\mathcal{L}_0|W_{\mathbf{k}}\rangle = E_{\mathbf{k}}|W_{\mathbf{k}}\rangle \quad (18)$$

and $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is the first Pauli matrix. Note that to the first order in \tilde{n}/n_c the thermal-cloud-induced corrections to the mode energies read

$$\Delta E_{\mathbf{k}} = \langle W_{\mathbf{k}} | \Delta \mathcal{L}_c^{(0)} + \Delta \tilde{\mathcal{L}}_{D=0}^{(0)} - \Delta \mu \sigma_3 | W_{\mathbf{k}} \rangle . \quad (19)$$

To define the frequency shift (15) in an excitation experiment one should know the stationary part $\tilde{\mathcal{L}}_{D=0}^{(0)}$ of the non-condensed corrections to the condensate Liouvillian and the “dynamical polarizability” $\frac{\partial}{\partial D} \Delta \tilde{\mathcal{L}}_{D=0}^{(-/+)}$. In general such a calculation would require a detailed knowledge of the dynamical response of all the thermal modes and it is a complicated numerical problem. However in some cases the calculation can be simplified: that is, for example, the case of an accidental degeneracy between the condensate oscillation frequency $\omega_{\mathbf{k}_{\text{mode}}}$ and one of the eigenfrequencies of the thermal cloud $\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1}$:

$$\omega_{\mathbf{k}_{\text{mode}}} \approx \omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1} . \quad (20)$$

In this case the time evolution of the cloud gets dominated by the two resonant modes (1 and 2) and the thermal cloud can be treated in a kind of *resonant approximation*, where only two modes evolve with time. The latter assumption is justified for the case of the “ $m = 2$ ” excitation experiment at JILA where the frequency of the mode of interest $\omega_{\mathbf{k}_{\text{mode}}} = \omega_{n=0,m=+2} \approx 1.45 \omega_p$ turns out to be close to the differential frequency $\omega_{\mathbf{k}_2} - \omega_{\mathbf{k}_1} = \omega_{n=2,m=+1}^{[-]} - \omega_{n=0,m=-1} \approx 1.65 \omega_p$ (mode classification corresponds to one suggested in [16]).

At this point we have to chose a specific model to describe the evolution of the thermal cloud: in what follows we will treat the thermal particles using a time-dependent Hartree-Fock-Bogoliubov approximation [8]. Under this approximation the evolution of the variance $\delta\hat{\psi} = \hat{\psi} - \langle \hat{\psi} \rangle$ of the bosonic field will be governed by a mean-field equation

$$\hbar \frac{\partial}{\partial t} \delta\hat{\psi} = [\frac{p^2}{2M} + V_{\text{trap}} + 2g(n_c + \tilde{n})] \delta\hat{\psi} + g(m_c + \tilde{m}) \delta\hat{\psi}^\dagger . \quad (21)$$

Furthermore we will suppose that prior to the excitation the system was in a thermal equilibrium.

Following the “resonant approximation” program described above one can show that in the resonant case the evolution of the thermal cloud is governed by a simple equation for an effective two-level atom in a resonant field of a Rabi frequency

$$\hbar \Omega_{\text{Rabi}} / 2 = 2gN_c \langle W_{\mathbf{k}_2} | \{(\sigma_3 \Phi) \otimes W_{\mathbf{k}_{\text{mode}}} \} | W_{\mathbf{k}_1} \rangle D + \mathcal{O}(D^2) \quad (22)$$

and detuning

$$\hbar \delta = \hbar \epsilon - [(E_{\mathbf{k}_2} + \Delta E_{\mathbf{k}_2}) - (E_{\mathbf{k}_1} + \Delta E_{\mathbf{k}_1}) - E_{\mathbf{k}_{\text{mode}}}] + \mathcal{O}(D) , \quad (23)$$

where the energy shifts $\Delta E_{\mathbf{k}}$ are given by (19) and the tensor product $\{\cdot \otimes \cdot\}$ is defined as

$$\begin{aligned} & \{W_p \otimes W_q\} \\ &= \begin{pmatrix} [U_p^* U_q + V_p^* V_q] & V_p^* U_q \\ -U_p^* V_q & -[U_p^* U_q + V_p^* V_q] \end{pmatrix} . \end{aligned} \quad (24)$$

We can identify two distinct classes of small collective excitations of the system: for the excitations of the first class (\downarrow) the stationary part of the thermal cloud is the same as in thermodynamic equilibrium prior to the beginning of the excitation process; for the second class (\uparrow) the populations of the two resonant modes are inverted with respect to the thermal equilibrium.

The thermal Liouvillian components (12, 17) we are interested in now read

$$\begin{aligned} \Delta \tilde{\mathcal{L}}_{D=0}^{(0)} &= \Delta \tilde{\mathcal{L}}_{\text{equilib.}} \\ &+ 2g(N_{\mathbf{k}_1} - N_{\mathbf{k}_2})(\{W_{\mathbf{k}_2} \otimes W_{\mathbf{k}_2}\} - \{W_{\mathbf{k}_1} \otimes W_{\mathbf{k}_1}\}) \\ &\times \left(\frac{w+1}{2} \right) \end{aligned} \quad (25)$$

$$\begin{aligned} \frac{\partial}{\partial D} \Delta \tilde{\mathcal{L}}_{D=0}^{(-/+)} &= 2g(N_{\mathbf{k}_1} - N_{\mathbf{k}_2})\{W_{\mathbf{k}_1} \otimes W_{\mathbf{k}_2}\} \\ &\times \left(\frac{\partial}{\partial D} \rho_{21} \right) , \end{aligned} \quad (26)$$

where

$$w = \begin{cases} -1, & \text{for the } (\downarrow)\text{-mode} \\ +1, & \text{for the } (\uparrow)\text{-mode} \end{cases} \quad (27)$$

is the population inversion;

$$\rho_{21} = -\Omega_{\text{Rabi}} w / 2\delta \quad (28)$$

is the coherence induced between mode 2 and mode 1; $N_{\mathbf{k}} = \{\exp(E_{\mathbf{k}}/T) - 1\}^{-1}$ are the Bose-Einstein occupation numbers in the thermal equilibrium; $\Delta \tilde{\mathcal{L}}_{\text{equilib.}} = ((2g\tilde{n}_{\text{equilib.}}, g\tilde{m}_{\text{equilib.}}), (-g\tilde{m}_{\text{equilib.}}^*, -2g\tilde{n}_{\text{equilib.}}))$ is the thermal cloud induced correction to the Bogoliubov-de-Gennes Liouvillian (9) calculated in the state of thermal equilibrium. Notice that we have preserved the first order in \tilde{n}/n_c terms in the denominator of the expression for the detuning (23), though this seems to contradict the expansion procedure we have chosen. In the *resonant* case, however, the presence of this terms is well justified since in this case the mean-field shifts $\Delta E_{\mathbf{k}}$ and the frequency shift ϵ can approach the “zeroth order” splitting $E_{\mathbf{k}_2} - E_{\mathbf{k}_1} - E_{\mathbf{k}_{\text{mode}}}$.

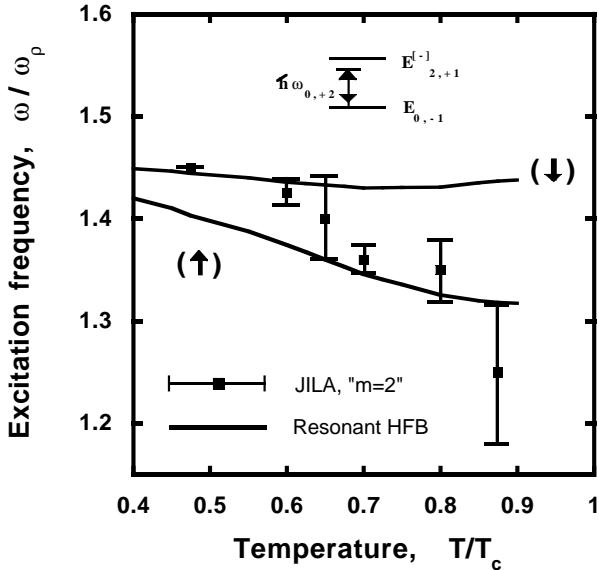


FIG. 1. Shift of the frequency of the “ $m=2$ ” collective excitation with respect to its zero-temperature value as a function of temperature. Lines show the collective modes we have found. Down(up) arrow corresponds to the normal(inverted) mode. Errorbars show JILA experimental data [2]. As a unit of frequency the radial trap frequency ω_p has been chosen. The inset illustrates the relationship between the energies of the modes involved in the model.

The formula for the frequency shift (15) along with those for the corrections to the Bogoliubov-de-Gennes Liouvillian (16,25) and dynamical polarizability of the thermal cloud (26) provides us with a closed implicit system of algebraic equations from which one can extract the values of the finite-temperature resonant corrections to the oscillations frequencies of the condensate. At the Fig.1 we show a comparison of our predictions with the experimental measurement of the “ $m=2$ ” condensate frequencies at JILA. We would suppose that in the temperature range below $T \sim .65 T_c$ the “normal” mode was excited in the experiment, whereas above this temperature the experimental points correspond to the “inverted” mode. The point at $T \sim .65 T_c$ can be associated with any of the two modes or, probably, with a superposition of them.

In our calculations the condensate wave-function Φ , “lost vector” Φ_a , chemical potential μ , and thermal-cloud-induced correction to the condensate wave-function $\Delta\Phi$ were described within the Thomas-Fermi approximation. The mode functions $|W_{\mathbf{k}_{\text{mode}}}\rangle = |W_{n=0,m=+2}\rangle$, $|W_{\mathbf{k}_1}\rangle = |W_{n=0,m=-1}\rangle$, and $|W_{\mathbf{k}_2}\rangle = |W_{n=2,m=+1,[-]}\rangle$ were approximated by the Thomas-Fermi expressions presented in [16]. For the mode energies we were using the finite- N numerical values calculated in [17], as the effect we are describing is very sensitive to the actual value of the energy splittings. Throughout our calculations we were neglecting the thermal equilibrium part $\Delta\tilde{\mathcal{L}}_{\text{equilib}}$ of the Liouvillian as this type of perturbation has been shown to have no significant effect in the frequency shifts

[5].

As we pointed out above, one of our collective modes corresponds to the inversion of populations of the thermal modes 1 and 2. Whether such an inversion can be reached in the experiment depends on details of the excitation procedure. We have checked, however, that the 3% amplitude variation of the trap frequency used in the JILA experiment is a strong saturating perturbation of the transition between the $\{n = 0, m = -1\}$ and $\{n = 2, m = +1, [-]\}$ thermal modes, and, therefore, the “inverted” mode could, indeed, be excited during the excitation stage. The answer of the question on which particular mode will be excited at a given temperature would involve a time-dependent analysis of the whole experimental sequence: it is a subject of our future research.

Two conclusions can be drawn from our work: (a) At finite temperatures the spectrum of the *collective* excitations of the condensate is essentially different from the spectrum of the *elementary* excitations, in contrary to the zero-temperature case. Comparison of the expressions (15) and (19) for the finite-temperature corrections to the former and latter shows that the collective excitation shift contains an extra term proportional to the “dynamical polarizability” of the thermal cloud; (b) Quantization of motion of the thermal quasi-particles is important and it can lead to significant effects, at least in the resonant case described in our paper.

Note also, that in the off-resonant limit our results are consistent with the conclusions of the work [8].

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